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Impact of Dynamic Orbital Correlations on Magnetic Excitations in the Normal State of Iron-Based Superconductors

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We show here that orbital degrees of freedom produce a distinct signature in the magnetic excitation spectrum of iron-based superconductors above the magnetic ordering temperature. Because d_{xz} and d_{yz} orbitals are strongly connected with the Fermi surface topology, the nature of magnetic excitations can be modified significantly due to the presence of either static or fluctuating orbital correlations. Within a five-orbital itinerant model, we show that static orbital order generally leads to an enhancement of commensurate magnetic excitations even when the original Fermi surface lacks nesting at $(\pi, 0)$ or $(0, \pi)$. When long-range orbital order is absent, Gaussian fluctuations beyond the standard random-phase approximation (RPA) capture the effects of fluctuating orbital correlations on the magnetic excitations. We find that commensurate magnetic excitations can also be enhanced if the orbital correlations are strong. Our results offer a natural explanation for the incommensurate-to-commensurate transformation observed in a recent neutron scattering measurement (Z. Xu, et. al., arXiv:1201.4404), and we propose that this unusual transformation is an important signature to distinguish orbital from spin physics in the normal state of the pnictides. Implications for the magnetic and superconducting states are discussed.

PACS numbers:

I. INTRODUCTION

Orbital-dependence of Fermi surface pockets due to the partial occupancy of multiple d-states of iron is a key microscopic feature which distinguishes iron-based supercondcutors from the cuprates. It is natural then that both orbital and spin-based scenarios have been advanced to account for the structural and magnetic transitions in these materials. In the orbital-based scenario[1–6], the structural phase transition is induced by a spontaneous orbital order in the quasi-one-dimensional d_{xz} and d_{yz} orbitals which breaks the C_4 symmetry. Such order induces a stripe-like antiferromagnetic (AFM) transition at a lower temperature.

By contrast, some have proposed that a spin-only model accounts for both the structural and magnetic transitions in the pnictides. While the source of the interactions that drive the magnetism differ in the strong-coupling[7–10] and weak-coupling[11–13] models proposed, both spin-based scenarios eventually end up with the same effective theory[13] with a magnetic order parameter lying in the manifold of $Z_2 \times O(3)$. The structural phase transition is interpreted as a breaking of the Z_2 symmetry, and the subsequent stripe-like AFM breaks $O(3)$ symmetry. The main difficulty in deciphering between these two scenarios is that both lead to the same Ginzburg-Landau effective action.

Although intensive research efforts has focused on the spin excitation spectrum in stripe-like AFM[14–16] and superconducting[17–19] states, a theoretical study on the effect of orbital order and fluctuations on the spin excitation spectrum in the paramagnetic normal state is far from complete. It is this problem that we tackle here. Our line of reasoning is based on the fact that if the spin interaction is the only energy scale driving both phase transitions, the difference in magnetic excitations between the normal and ordered states should be tied solely to a redistribution of spectral weight. The positions of the peaks in the Brillouin zone, namely the magnetic spectrum, should not undergo any qualitative change. On the other hand, if there is an additional energy scale playing an equally important role, then this extra energy scale could result in qualitatively distinct changes in the magnetic spectrum above and below the ordering transition.

In this paper, we analyse the magnetic excitations within a five-orbital itinerant model with generalized on-site Hubbard interactions. and superconducting[17–19] states, Since our main purpose is to identify several features which can not be captured without involving orbital degrees of freedom, an orbital-dependent non-spin interaction is introduced in order to investigate systematically how orbital correlations affect the magnetic excitations in the paramagnetic normal state. We find that orbital order always enhances one of the commensurate spin excitation wave vectors even when the original Fermi surfaces lack nesting at these commensurate wave vectors. Moreover, to include the effect of fluctuating orbital correlations on the magnetic excitations, we derive a Gaussian fluctuation model to go beyond the standard random-phase approximation (RPA) treatment. Even in this case, we find that fluctuating orbital correlations also tend to shift the spectral weight toward the commensurate wave vector, resulting in a broad spectrum near the commensurate wave vectors as seen in neutron scattering measurements. We show that our results offer a natural explanation for the incommensurate-to-commensurate transformation observed in the inelastic neutron scat-

tering measurement on $Fe_{1-x}Ni_xTe_{0.5}Se_{0.5}$[20], which can hardly be explained by spin-based scenarios. As there is no reason to suspect that one model is insufficient to explain the normal state of the pnictides, we conclude that orbital physics is the key player in driving both the structural as well as the magnetic transitions in the iron-based superconductors. We propose further experimental studies on magnetic excitations at higher temperature in the normal state to further pin down the orbital scenario.

II. FORMALISM

A. Random phase approximation (RPA) theory for the magnetic excitation

Starting from a tight-binding model in the unfolded Brillouin zone with one Fe atom per unit cell, we write the model Hamiltonian as

$$H = H_t + H_{OO} + H_I$$
$$H_I = \sum_{ia} U n_{ia\uparrow} n_{ia\downarrow} + \sum_{i,b>a} (U' - \frac{J}{2}) n_{ia} n_{ib}$$
$$- \sum_{i,b>a} 2J \vec{S}_{ia} \cdot \vec{S}_{ib} + J'(p_{ia} p_{ib}^\dagger + h.c.), \quad (1)$$

where

$$n_{ia} \equiv \sum_\sigma c_{ia\sigma}^\dagger c_{ia\sigma},$$
$$\vec{S}_{ia} \equiv c_{ia\mu}^\dagger \vec{\sigma}_{\mu,nu} c_{ia\sigma\nu},$$
$$p_{ia} \equiv c_{ia\downarrow} c_{ia\uparrow}. \quad (2)$$

We adopt the relationships $U' = U - 2J$, $J = J'$ and throughout the paper we use the values of $U = 2.0eV$ and $J = 0.2eV$. H_t is the five-orbital tight-binding model fitted by Graser *et. al.*[18], and H_{OO} is the effective interaction for 'orbital order' which we put in by hand as

$$H_{OO} = \frac{1}{N} \sum_{\vec{q}} \eta_q \zeta_{-\vec{q}} \zeta_{\vec{q}}$$
$$\zeta_{\vec{q}} = \sum_{\vec{k},\sigma} (c_{xz,\sigma}^\dagger(\vec{k}+\vec{q}) c_{xz,\sigma}(\vec{k}) - c_{yz,\sigma}^\dagger(\vec{k}+\vec{q}) c_{yz,\sigma}(\vec{k})). \quad (3)$$

We do not justify the microscopic origin of H_{OO} since the conclusion is independent of the mechanism for orbital order. However, we will comment on the differences in the magnetic excitations for different scenarios in the discussion section. For ferro-orbital order, we have $\eta_q = -\eta_0$ for $\vec{q} = 0$, which leads to a mean-field Hamiltonian of the form,

$$H^{MF} = H_t - \phi \sum_{\vec{k},\sigma} (c_{xz,\sigma}^\dagger(\vec{k}) c_{xz,\sigma}(\vec{k}) - c_{yz,\sigma}^\dagger(\vec{k}) c_{yz,\sigma}(\vec{k})) \quad (4)$$

with $\phi = \frac{\eta_0}{N}\langle\zeta_{\vec{q}=0}\rangle$ solved self-consistently. It is convenient to use the basis, $\psi_{\vec{k},\sigma}^\dagger \equiv (c_{\vec{k},xz,\sigma}^\dagger, c_{\vec{k},yz,\sigma}^\dagger, c_{\vec{k},xy,\sigma}^\dagger, c_{\vec{k},x^2-y^2,\sigma}^\dagger, c_{\vec{k},3z^2-r^2,\sigma}^\dagger)$, and introduce $\hat{U}_{\vec{k}}^\sigma$ such that $(\hat{U}_{\vec{k}}^\sigma)^\dagger \hat{H}^{MF}(\vec{k},\sigma)\hat{U}_{\vec{k}}^\sigma = \text{diag.}[E_{\vec{k},1,\sigma}, \cdots, E_{\vec{k},5,\sigma}]$. It then follows that the bare response function can be expressed as

$$\chi_{ab;cd}^{(0)}(\vec{q}, i\omega_n, \phi)$$
$$= -\frac{1}{N} \sum_{\vec{k},\sigma,l,m} (\hat{U}_{\vec{k}+\vec{q}}^\sigma)_{a,l} (\hat{U}_{\vec{k}+\vec{q}}^\sigma)_{c,l}^* (\hat{U}_{\vec{k}}^\sigma)_{d,m} (\hat{U}_{\vec{k}}^\sigma)_{b,m}^*$$
$$\times \frac{n_F(E_{\vec{k}+\vec{q},l,\sigma}) - n_F(E_{\vec{k},m,\sigma})}{E_{\vec{k}+\vec{q},l,\sigma} - E_{\vec{k},m,\sigma} - i\omega_n}. \quad (5)$$

Using the same notation as Graser *et. al.*[18], we express the spin response function to one-loop as

$$\chi^{RPA}(\vec{q},\omega,\phi) = \chi^{(0)}(\vec{q},\omega,\phi)[1 - \hat{V}^s \chi^{(0)}(\vec{q},\omega,\phi)]^{-1} \quad (6)$$

where $\hat{V}^s$ is the spin interaction kernel derived in Ref.[19].

B. Gaussian fluctuations in the absence of long-range order

Even above the transition for long-ranged orbital order, the magnetic excitations can still be influenced by the fluctuations in the proximity to the orbitally ordered state. In this section, the minimal Gaussian fluctuation model is derived from the path integral formalism. Since our focus is on the interplay between spin-flip excitations and orbital ordering in the normal state without any long-range order, we introduce the Hubbard-Stratonovich fields to decouple H_{OO} and the spin-flip channels in H_I

$$S_{ab}^+(\vec{q}) \equiv \sum_{\vec{k}} c_{\vec{k}+\vec{q},a,\uparrow}^\dagger c_{\vec{k},b,\downarrow}, \quad (7)$$

and drop all the other terms. The partition function takes the form,

$$Z = \int D[c]D[c^\dagger]e^{-S_0-S_I-S_{OO}}$$
$$\propto \int D[\phi]D[\phi^*]D[M]D[M^*]D[c]D[c^\dagger]e^{-S_0-S_M+S'_{OO}}$$
$$S_M = \sum_{\vec{k},\vec{q},i\omega_n} \sum_{abcd} [M_{ab}(\vec{q},i\omega_n)S_{cd}^-(\vec{q},i\omega_n)$$
$$+ M_{ab}(-\vec{q},-i\omega_n)S_{cd}^+(\vec{q},i\omega_n)$$
$$+ [\hat{V}^s]_{ab,cd}^{-1}(\vec{q},i\omega_n)M_{ab}(-\vec{q},-i\omega_n)M_{cd}(\vec{q},i\omega_n)]$$
$$S'_{OO} = \sum_{\vec{q},i\omega_n} [\phi(\vec{q},i\omega_n)\zeta(-\vec{q},-i\omega_n) + \phi(-\vec{q},-i\omega_n)\zeta(\vec{q},i\omega_n)$$
$$+ \eta_q^{-1}\phi^*(-\vec{q},-i\omega_n)\phi(\vec{q},i\omega_n)]. \quad (8)$$

Because we are interested in the case where the system is on the verge of ferro-orbital order but not close to any instability in spin channel, the largest weight in the partition function comes from the Gaussian fluctuations around $(\vec{q} = 0, i\omega_n = 0)$ in the ϕ field. Therefore, we keep only the $\phi(\vec{q} = 0, i\omega_n = 0)$ field in Eq. 8 and treat the spin part by the standard saddle point approximation. After integrating out the fermionic fields and expanding all the Hubbard-Stratonovich fields up to quadratic order, we arrive at a partition function of the form,

$$Z \approx \int D[\phi(0)]D[\phi(0)^*]D[M]D[M^*]e^{-S_m-S_{oo}}$$
$$S_m = \sum_{\vec{k},\vec{q},i\omega_n} [\chi^{RPA}]^{-1}_{ab,cd}(\vec{q}, i\omega_n, \phi(0))$$
$$\times M_{ab}(-\vec{q}, -i\omega_n)M_{cd}(\vec{q}, i\omega_n)]$$
$$S_{oo} = \lambda^{-2}\phi^*(0)\phi(0), \tag{9}$$

where $\lambda^{-2} = \eta_0^{-1} - \Pi(\vec{q} = 0, i\omega = 0)$ is the stiffness for $\phi(0)$ field renormalized by the bubble diagrams. Then it is straightforward to arrive at the spin response function with minimal Gaussian fluctuations:

$$\chi^{Gaussian}(\vec{q}, \omega) = \frac{\int d\phi e^{-\phi^2/\lambda^2}\chi^{RPA}(\vec{q}, \omega, \phi)}{\int d\phi e^{-\phi^2/\lambda^2}} \tag{10}$$

where λ^2 is an effective parameter measuring the strength of the fluctuating orbital correlations. The physical meaning of the above Gaussian fluctuation model is clear. Because the system is on the verge of the ferro-orbital order, the fluctuations of the ϕ fields at $(\vec{q} = 0, i\omega_n = 0)$ is dominant. Either quantum or thermal fluctuations can create a temporary ferro-orbital order with a probability of $e^{-\phi(0)^2/\lambda^2}$, which is the leading fluctuating orbital correlations in this case. It is worth mentioning that the orbital order parameter $\langle\phi\rangle = 0$ is strictly fulfilled so that there is no long-range order. This is analogous to the formalism used by Gollub *et. al.* to study diamagnetism above T_c in conventional superconductors[22].

III. RESULTS

Our main results are summarized in Figs. 1, 2, and 4. The imaginary part of the spin susceptibility is plotted along the direction transvers to the $\vec{Q}_{AFM} = (\pi, 0)$ for different cases. From Figs. 1(a)-(c), it can be seen clearly that with the increase of the orbital order parameter, the peaks in the magnetic excitation gradually move from incommensurate to commensurate wave-vectors, which can be understood solely in terms of the Fermi surface topology. Generally speaking, the realistic Fermi surfaces of the iron-based superconductors does not have perfect nesting at $(\pi, 0)$ and $(0, \pi)$, and previous calculations have shown that in the normal state, the peaks in the spin susceptibility are usually incommensurate away from $(\pi, 0)$, $(0, \pi)$[16,18,21,23]. However, due to the presence
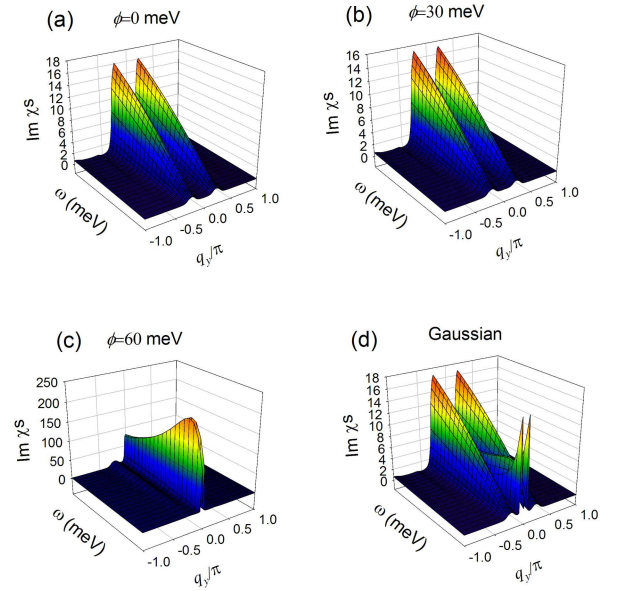

FIG. 1: The imaginary part of the spin susceptibility are plotted along $\vec{q} = (\pi, q_y)$ for (a) $\phi = 0$, (b) $\phi = 30$ meV, (c) $\phi = 60$ meV, and (d) Gaussian fluctuations with $\lambda^2 = 60$ meV. In this figure, the chemical potential μ is set to be 0 in the tight-binding model proposed in Ref.[18], corresponding to an electron doping of about 5%.

of orbital order, the Fermi surfaces are distorted along one of the in-plane axes, which always helps the enhancement of the magnetic excitations at $(\pi, 0)$ for $\phi > 0$ (or $(0, \pi)$ for $\phi < 0$). It follows then that the stripe-like antiferromagnetism accompanying pre-existing orbital order should have $\vec{Q}_{AFM} = (\pi, 0)$ for $\phi > 0$ or $\vec{Q}_{AFM} = (0, \pi)$ for $\phi < 0$, which has been confirmed by previous meanfield[24] and first principle calculations[3].

The magnetic excitations are also strongly modified without long-range orbital order but with fluctuating orbital correlations. In this case, because the fluctuating orbital correlations induce fluctuations of the Fermi surface shape, the magnetic excitations at the incommensurate wave vectors are significantly diffused toward the commensurate ones. This results in a broadened spectrum near $(\pi, 0)$, which can be seen from the results of our Gaussian fluctuation model shown in Fig. 1(d). The imaginary part of the spin susceptibility are plotted for different doping level in Fig. 2, which shows the same behavior.

It is remarkable to see that our results offer a natural explanation for several puzzles present in previous inelastic neutron scattering measurements. As shown in Fig. 3, for superconducting $Fe_{1-x}Ni_xTe_{0.5}Se_{0.5}$ with $x = 0.04$, the overall shape of the magnetic excitations at low energy udergoes a distinct transformation from two incommensurate vertical coloumns to a broad U-shaped spectrum centered at the commensurate wave vectors. As shown in Ref. [20], the change occurs at $T_{onset} \sim 3T_c$. Although we can not obtain the temperature-dependence
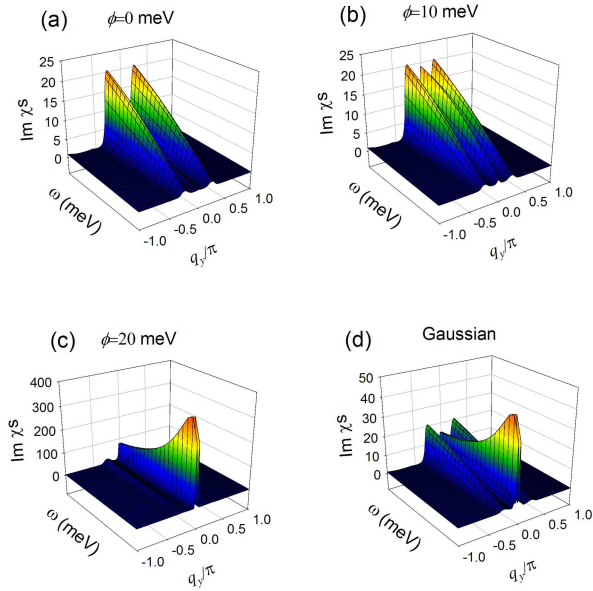
FIG. 2: The imaginary part of the spin susceptibility are plotted for doping level about 9% for (a) $\phi = 0$, (b) $\phi = 10$ meV, (c) $\phi = 20$ meV, and (d) Gaussian fluctuations with $\lambda^2 = 30$ meV.

FIG. 3: Inelastic neutron scattering measurement (data from Xu *et. al.*[20]) of $Fe_{1-x}Ni_xTe_{0.5}Se_{0.5}$ with $x = 0.04$ along the transverse direction to Q_{AFM} for (a) high temperature normal state ($T > T_{fluc}$) and (b) the superconducting state ($T < T_c$). An incommensurate-to-conmmensurate transformation is observed as the sample is cooled down.

of λ^2 from a microscopic calculation within the current model, it is expected that λ^2 should gradually increase if the system gets closer to the orbitally ordered state as the temperature is lowered. Consequently, this unusual incommensurate-to-commensurate transformation can be captured by our theory, as shown in Fig. 4, if we identify T_{onset} as the onset temperature of the fluctuating orbital correlations T_{fluc}. Moreover, a weak lattice distortion has been found in x-ray measurements[20,25], which gives further support for our orbital-based explanation.

Another interesting observation pointed out by Ewings *et. al.*[21] in inelastic neutron scattering measurement for $SrFe_2As_2$ is that after a thorough comparison between experimental data and theories, the multiorbital itinerant model treated with RPA[16] captures more details of the experimental data compared to a local moment model, except the theory obtained an incommensurate spectrum in the normal state which is not seen in experiments. This inconsistency can be easily resolved by the inclusion of the Gaussian fluctuation model presented in this paper. As seen in Fig. 4, while the incommensurate peaks for $T > T_{fluc}$ similar to Ref. [16] are reproduced in our calculations, the spectral weights of these incommensurate peaks are gradually shifted to $(\pi, 0)$ as the static and fluctuating orbital correlations are taken into account. Another subtle point worthy of mentioning is that there is no soft mode at $\vec{q} = (\pi, \pi)$ in our results, which is an important advantage of itinerant model over local moment model as mentioned in Ref. [21].
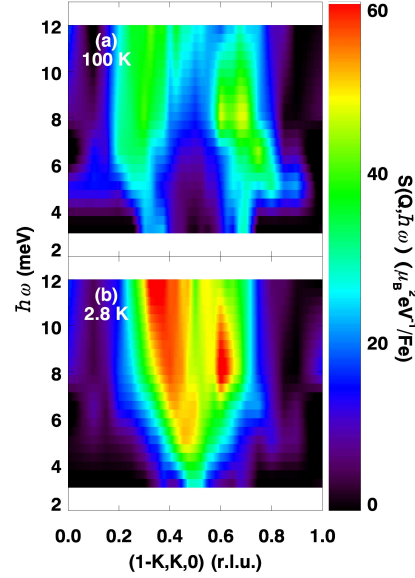
IV. DISCUSSION

First, we would like to discuss the nature of the magnetic excitations in spin-based scenarios proposed for iron-based superconductors. For the local spin scenario with frustrating J_1-J_2 interactions, it is generally hard to obtain peaks at incommensurate wave vector in the spin excitation spectrum in the paramagnetic state. One possibility is to include more longer-range spin interactions (e.g., J_3)[26]. Even so, it would be difficult to understand why the system would start from an incommensurate spin excitation spectrum at high temperature and then evolve into a stripe-like AFM with a commensurate wave vector. For the SDW scenario, there are only incommensurate magnetic excitations in the high temperature normal state, as seen in Ref. [20], and hence this model is not applicable. As a result, we conclude that the incommensurate-to-commensurate transformation in the magnetic excitations is a unique signature favoring orbital-based over spin-based scenarios. However, we also recognize the fact that the size of the instantaneous moments is too large to be described by a purely itinerant model in all current existing neutron scattering data. This suggests that one needs to take into account the orbital correlations emerging from an itinerant model to get the spin interactions correctly. Further inelastic neutron scattering measurements in the high temperature normal state are certainly necessary to resolve the long-standing controversy between the orbital-based and
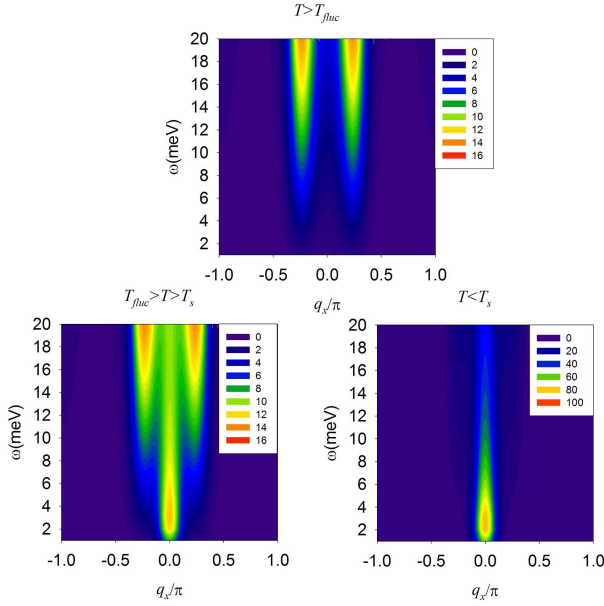
FIG. 4: Demonstration of the evolution of the imaginary part of the spin susceptibility along $\vec{q} = (\pi, q_y)$ as the temperature is lowered from high temperature. The parameters in the tight-binding model are the same as Fig. 1, and a broadening in the $\vec{q}$-space of $q_0 = 0.1\pi$ is introduced with the form of $\mathrm{Im}\chi^B(\vec{q}, \omega) = \sum_{\vec{q}'} e^{-(\vec{q}-\vec{q}')^2/q_0^2} \mathrm{Im}\chi(\vec{q}', \omega)/\sum_{\vec{q}'} e^{-(\vec{q}-\vec{q}')^2/q_0^2}$ for the ease of comparison with the experimental data in Fig. 3. For $T > T_{fluc}$, orbital fluctuations do not affect the magnetic excitations. In this case, H_{OO} is completely turned off. For $T_{fluc} > T > T_s$, the system does not have long-range orbital order but rather has fluctuating orbital correlations, which can be described at the Gaussian level (in the plot, $\lambda^2 = 30$ meV is used). For $T < T_s$, an orbital order is formed and the magnetic excitation is commensurate. The orbital order parameter in the plot is $\phi = 20$ meV.

spin-based scenarios.

Second, we comment briefly on materials. FeSe is a known iron-based superconductor exhibiting only a structural transition and no magnetic transition[27,28] and hence is a promising prototype for the orbital-based scenario as well as the incommensurate-to-commensurate transformation in its magnetic excitation spectrum. The families of iron-based superconductors whose structural and magnetic transition temperatures are well-separated, including LaOFeAs[29], CeOFeAs[30], NaFeAs[31–34], etc., should also be good candidates to realize the physics outlined in this paper. There have been neutron scattering measurements for parent compounds of 122, for example, $BaFe_2As_2$[35], $CaFe_2As_2$[36,37], and $SrFe_2As_2$[21], and interestingly they show very different trends. While the magnetic excitations in $CaFe_2As_2$ can be well-described by the local spin scenario both in the magnetic and the normal states, itinerant models seems to work better in $BaFe_2As_2$ and $SrFe_2As_2$. As suggested in Ref. [21], the reason why the local spin scenario fails in $SrFe_2As_2$ is that in the high temperature normal state, the magnetic excitations at momentum (π, π) are pushed to high energy which clearly contradicts the prediction of the local spin scenario unless one accepts that the anisotropic spin interactions can still be present even above the magnetic transitions. The most serious problem with the itinerant model for $SrFe_2As_2$ is the prediction of an incommensurate excitation spectrum in the high temperature normal state. This can be resolved with the Gaussian fluctuating orbital correlations proposed here. In other words, in order to explain the neutron scattering data of $SrFe_2As_2$, the orbital degrees of freedom are necessary even in a spin-based scenario. Therefore, since the previous work on $BaFe_2As_2$ only measured up to 150K, slightly above the magnetic transition temperature ($\sim$ 140K), it would be essential to perform further neutron scattering measurement at much higher temperature to see whether or not the features observed in $SrFe_2As_2$ appear in $BaFe_2As_2$. Should they be observed, this would further substantiate the orbital-based physics proposed here.

Third, we discuss the implication of our theory for superconductivity. Since most iron-based superconductors require doping away from the parent compounds to induce superconductivity, this strongly suggests that the Fermi surfaces of superconducting samples generally do not have perfect nesting at $(\pi, 0)$ and $(0, \pi)$. Consequently, if the pairing mechanism of the iron-based superconductors is really through spin fluctuations[18,23], the necessary commensurate spin excitation in this mechanism can not be obtained without the fluctuating orbital correlations discussed in this paper. This implies that the role of the orbital degrees of freedom in the superconductivity in the iron-based superconductors might be very profound. Recently, orbital-dependent superconducting gaps have been observed in the superconducting $Ba_{1-x}K_xFe_2As_2$ via Laser ARPES measurement[38]. The electronic structure of the vortex core in the FeSe superconductors shows a strong anisotropy[39], which has been interpreted as a consequence of competition between nematicity (orbital order) and superconductivity[40,41]. A very recent ARPES measurement[42] revealed that the doping dependence of the band renormalizations of d_{xz} and d_{yz} orbitals strongly correlate with the enhancement of the superconductivity. These new findings strongly suggest that only an inceptive understanding of superconductivity would obtain without including the orbital degree of freedom. We propose that the incommensurate-to-commensurate transformation in the magnetic excitations should be a general feature in most superconducting iron pnictides.

Finally, we would like to discuss the magnetic excitation along the direction longitudinal to Q_{AFM}. Our model showed that the magnetic excitation still disperses along this direction, despite the fact that the spectral weight could be different from that along the transverse direction. Experimentally, it has been found that the magnetic dispersion is absent along the longitudinal direction for FeTe/Se systems[20,43], which remains a puzzle

and is beyond our current model. One possibility is to exploit an effective degenerate double exchange model[5] whose spin interactions are orbital dependent so that the effects of the orbital correlations discussed in this paper could be correctly incorporated. This work is currently under development.

V. CONCLUSION

In this paper, we have studied magnetic excitations in the normal state of the iron based superconductors. Because the orbitals of d_{xz} and d_{yz} are closely related to the shape of the Fermi surface, orbital order which distorts the Fermi surfaces, can have a profound effect on the magnetic excitations. We do not specify the origin of the orbital ordering and fluctuations since the results are generally valid regardless of the origin. Furthermore, we assume that the ferro-orbital fluctuations are the dominating ones as the structure phase transition is approached from higher temperature. We have shown that orbital order always enhances one of the commensurate spin excitation wave vector even when the original Fermi surfaces do not have a nesting at these commensurate wave vectors. Furthermore, even when long-range orbital order is absent, Gaussian fluctuations of the orbital order can still couple to the magnetic excitations. We found that these Gaussian fluctuations also tend to diffuse the spectral weights toward the commensurate wave vector, resulting in a broad spectrum near the commensurate wave vectors as seen in neutron scattering measurements[20]. We have shown that this orbital-based scenario offers a natural explanation for the incommensurate-to-commensurate transformation observed in $Fe_{1-x}Ni_xTe_{0.5}Se_{0.5}$, which can hardly be explained by spin-based scenarios. We propose that this unusual transformation is an important signature that can distinguish orbital from spin-based physics in the pnictides. Our theory can be tested by further neutron scattering experiments at higher temperatures.

VI. ACKNOWLEDGMENTS

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